ELECTRONIC INFORMATION DISCLOSURE STATEMENT

Electronic Version v18
Stylesheet Version v18.0

Title of Invention	Method, System and Computer Program Product for Representing Object Relationships in a Multidimensional Space

Application Number: 09/823977
Confirmation Number: 9693
First Named Applicant: Dimitrus Agrafiotis
Attorney Docket Number: 1503.0930001
Search string: (5807754 or 5811241 or 5832494 or 5858660 or 5861532 or 5866334 or 5901069 or 5908960 or 5933819 or 6026397 or 6037135 or 6049797 or 6185506 or 6240374 or 6295514 or 6014661).pn.

US Patent Documents

Note: Applicant is not required to submit a paper copy of cited US Patent Documents

init	Cite.No.	Patent No.	Date	Patentee	Kind	Class	Subclass
	1	5807754	1998-09-15	Zambias et al.			
	2	5811241	1998-09-22	Goodfellow et al.			
	3	5832494	1998-11-03	Egger et al.			
	4	5858660	1999-01-12	Eaton et al.			
	5	5861532	1999-01-19	Brown et al.			
	6	5866334	1999-02-02	Beutel			
	7	5901069	1999-05-04	Agrafiotis et al.			
	8	5908960	1999-06-01	Newlander			
	9	5933819	1999-08-03	Skolnick et al.			
	10	6026397	2000-02-15	Sheppard			
	11	6037135	2000-03-14	Kubo et al.			
	12	6049797	2000-04-11	Guha et al.			
	13	6185506	2001-02-06	Cramer et al.	B1		
	14	6240374	2001-05-29	Cramer et al.	B1		
	15	6295514	2001-09-25	Agrafiotis et al.	B1		
	16	6014661	2000-01-11	Ahlberg et al.			

Signature

Examiner Name	Date
[signature]	24JAN04

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First Named Applicant: Dimitrus Agrafiotis
Attorney Docket Number: 1503.0930001
Search string: (4773099 or 4811217 or 4859736 or 4908773 or 4935875 or 4939666 or 5010175 or 5025388 or 5155801 or 5167009 or 5181259 or 5240680 or 5260882 or 5265030 or 5270170 or 5288514 or 5307287 or 5323471 or 5331573 or 5434796 or 5436850 or 5442122 or 5463564 or 5499193 or 5519635 or 5524065 or 5526281 or 5545568 or 5549974 or 5095443 or 5553225 or 5574656 or 5585277 or 5598510 or 5602755 or 5602938 or 5612895 or 5621861 or 5634017 or 5635598 or 5670326 or 5679582 or 5684711 or 5703792 or 5712171 or 5712564 or 5734796 or 5736412 or 5740326 or 5789160).pn.

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init	Cite.No.	Patent No.	Date	Patentee	Kind	Class	Subclass
	1	4773099	1988-09-20	Bokser			
	2	4811217	1989-03-07	Tokizane et al.			
	3	4859736	1989-08-22	Rink			
	4	4908773	1990-03-13	Pantoliano et al.			
	5	4935875	1990-06-19	Shah et al.			
	6	4939666	1990-07-03	Hardman			
	7	5010175	1991-04-23	Rutter et al.			
	8	5025388	1991-06-18	Cramer, III et al.			
	9	5155801	1992-10-13	Lincoln			
	10	5167009	1992-11-24	Skeirik			
	11	5181259	1993-01-19	Rorvig			
	12	5240680	1993-08-31	Zuckermann et al.			
	13	5260882	1993-11-09	Blanco et al.			
	14	5265030	1993-11-23	Skolnick et al.			
	15	5270170	1993-12-14	Schatz et al.			
	16	5288514	1994-02-22	Ellman			
	17	5307287	1994-04-26	Cramer, III et al.			
	18	5323471	1994-06-21	Hayashi			
	19	5331573	1994-07-19	Balaji et al.			
	20	5434796	1995-07-18	Weininger			

	21	5436850	1995-07-25	Eisenberg et al.
	22	5442122	1995-08-15	Noda et al.
	23	5463564	1995-10-31	Agrafiotis et al.
	24	5499193	1996-03-12	Sugawara et al.
	25	5519635	1996-05-21	Miyake et al.
	26	5524065	1996-06-04	Yagasaki
	27	5526281	1996-06-11	Chapman et al.
	28	5545568	1996-08-13	Ellman
	29	5549974	1996-08-27	Holmes
	30	5095443	1992-03-10	Watanabe
	31	5553225	1996-09-03	Perry
	32	5574656	1996-11-12	Agrafiotis et al.
	33	5585277	1996-12-17	Bowie et al.
	34	5598510	1997-01-28	Castelaz
	35	5602755	1997-02-11	Ashe et al.
	36	5602938	1997-02-11	Akiyama et al.
	37	5612895	1997-03-18	Balaji et al.
	38	5621861	1997-04-15	Hayashi et al.
	39	5634017	1997-05-27	Mohanty et al.
	40	5635598	1997-06-03	Lebl et al.
	41	5670326	1997-09-23	Beutel
	42	5679582	1997-10-21	Bowie et al.
	43	5684711	1997-11-04	Agrafiotis et al.
	44	5703792	1997-12-30	Chapman
	45	5712171	1998-01-27	Zambias et al.
	46	5712564	1998-01-27	Hayosh
	47	5734796	1998-03-31	Pao
	48	5736412	1998-04-07	Zambias et al.
	49	5740326	1998-04-14	Boulet et al.
	50	5789160	1998-08-04	Eaton et al.

Signature

Examiner Name	Date
[signature]	24 Jan 04

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0930001	APPLICATION NO. 09/823,977
	APPLICANT Agrafiotis *et al.*	RECEIVED
	FILING DATE April 3, 2001	GROUP 2122 MAY 30 2003

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA1						
	AB1						
	AC1						
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	AH1						
	AI1						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
W2	AJ1	EP 0 355 266 B1	02/1990	EPO	B01J	19/00	Yes No
	AK1	EP 0 355 628 B1	02/1990	EPO	G21F	9/00	Yes No
	AL1	EP 0 770 876 A1	05/1997	EPO	G01N	33/68	Yes No
	AM1	EP 0 818 744 A2	01/1998	EPO	G06F	17/50	Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

W2	AN	1	Borg, Ingwer and Groenen, Patrick, *Modern Multidimensional Scaling Theory and Applications*, Springer Series in Statistics, 1997, entire book submitted.
	AO	1	Agrafiotis, D.K. *et al.*, "Advances in diversity profiling and combinatorial series design," *Molecular Diversity*, Kluwer Academic Publishers, Vol. 4, 1999, pp. 1-22.
	AP	1	Agrafiotis, D.K. and Lobanov, V.S., "An Efficient Implementation of Distance-Based Diversity Measures Based on *k-d* Trees," *Journal of Chemical Information and Computer Science*, American Chemical Society, Vol. 39, No. 1, November 17, 1999 (Published on Web), pp. 51-58.
	AQ	1	Agrafiotis, D.K. and Lobanov, V.S., "Bridging The Gap Between Diversity And QSAR," *Abstracts of Papers Part 1: 215th ACS National Meeting*, American Chemical Society, March 29-April 2, 1998, p. 181-COMP.
	AR	1	Agrafiotis, D.K. and Jaeger, E.P., "Directed Diversity®: An Operating System For Combinatorial Chemistry," *Abstracts of Papers Part 1: 211th ACS National Meeting*, American Chemical Society, March 24-28, 1996, p. 46-COMP.

EXAMINER	DATE CONSIDERED
	24 JAN 04

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	AA2						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ2	WO 91/19735	12/1991	PCT	C07K	7/02	Yes No
	AK2	WO 92/00091	01/1992	PCT	A61K	37/02	Yes No
	AL2	WO 93/20242	10/1993	PCT	C12Q	1/70	Yes No
	AM2	WO 94/28504	12/1994	PCT	G06F	15/60	Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	2	Agrafiotis, D.K., "Diversity of Chemical Libraries," *Encyclopedia of Computational Chemistry*, John Wiley & Sons Ltd, Vol. 1:A-D, 1998, pp. 742-761.
	AO	2	Agrafiotis, D.K., "On the Use of Information Theory for Assessing Molecular Diversity," *Journal of Chemical Information and Computer Science*, American Chemical Society, Vol. 37, No. 3, May/June 1997, pp. 576-580.
	AP	2	Agrafiotis, D.K. *et al.*, "Parallel QSAR," *Abstracts of Papers Part 1: 217th ACS National Meeting*, March 21-25, 1999, p. 50-COMP.
	AQ	2	Agrafiotis, D.K. *et al.*, "PRODEN: A New Program for Calculating Integrated Projected Populations," *Journal of Computational Chemistry*, John Wiley & Sons, Inc., Vol. 11, No. 9, October 1990, pp. 1101-1110.
	AR	2	Agrafiotis, D.K. and Jaeger, E.P., "Stochastic Algorithms for Exploring Molecular Diversity," *Abstracts of Papers Part 1: 213th ACS National Meeting*, American Chemical Society, April 13-17, 1997, p. 16-CINF.

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	AA3						
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	AH3						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
WG	AJ3	WO 95/01606	01/1995	PCT	G06F	15/42	Yes No
	AK3	WO 97/09342	03/1997	PCT	C07H	21/02	Yes No
	AL3	WO 97/20952	06/1997	PCT	C12Q	1/68	Yes No
	AM3	WO 97/27559	07/1997	PCT	G06F	19/00	Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

WG	AN	3	Agrafiotis, D., "Theoretical Aspects of the Complex: Arts and New Technologies," *Applications and Impacts Information Processing '94*, North-Holland, Vol. II, 1994, pp. 714-719.
	AO	3	Biswas, G. *et al.*, "Evaluation of Projection Algorithms," *IEEE Transactions On Pattern Analysis And Machine Intelligence*, IEEE Computer Society, Vol. PAMI-3, No. 6, November 1981, pp. 701-708.
	AP	3	Bonchev, D. and Trinajstić, N., "Information theory, distance matrix, and molecular branching," *The Journal of Chemical Physics*, American Institute of Physics, Vol. 67, No. 10, November 15, 1977, pp. 4517, 4520-4533.
	AQ	3	Chang, C.L. and Lee, R.C.T., "A Heuristic Relaxation Method for Nonlinear Mapping in Cluster Analysis," *IEEE Transactions on Systems, Man, and Cybernetics*, IEEE Systems, Man, and Cybernetics Society, Vol. SMC-3, March 1973, pp. 197-200.
	AR	3	Cramer, R.D. *et al.*, "Virtual Compound Libraries: A New Approach to Decision Making in Molecular Discovery Research," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, Vol. 38, No. 6, November/December 1998, pp. 1010-1023.

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	AA4						
	AB4						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ4	WO 98/20437	05/1998	PCT	G06F	17/50	Yes No
	AK4	WO 98/20459	05/1998	PCT	G06T	11/20	Yes No
	AL4						Yes No
	AM4						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	4	DeMers, D. and Cottrell, G., "Non-Linear Dimensionality Reduction," *Advances in Neural Information Processing Systems*, Vol. 5, 1993, pp. 580-587.
	AO	4	Frey, P.W. and Slate, D.J., "Letter Recognition Using Holland-Style Adaptive Classifiers," *Machine Learning*, Kluwer Academic Publishers, Vol. 6, 1991, pp. 161-182.
	AP	4	Friedman, J.H., "Exploratory Projection Pursuit," *Journal of the American Statistical Association*, American Statistical Association, Vol. 82, No. 397, March 1987, pp. 249-266.
	AQ	4	Friedman, J.H. and Tukey, J.W., "A Projection Pursuit Algorithm for Exploratory Data Analysis," *IEEE Transactions on Computers*, IEEE Computer Society, Vol. C-23, No. 9, September 1974, pp. 881-889.
	AR	4	Garrido, L. *et al.*, "Use of Multilayer Feedforward Neural Nets As A Display Method for Multidimensional Distributions," *International Journal of Neural Systems*, World Scientific Publishing Co. Pte. Ltd., Vol. 6, No. 3, September 1995, pp. 273-282.

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	AA5						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ5						Yes No
	AK5						Yes No
	AL5						Yes No
	AM5						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	5	Ghose, A.K. *et al.*, "Prediction of Hydrophobic (Lipophilic) Properties of Small Organic Molecules Using Fragmental Methods: An Analysis of ALOGP and CLOGP Methods," *Journal of Physical Chemistry,* American Chemical Society, Vol. 102, No. 21, May 21, 1998, pp. 3762-3772.
	AO	5	Hall, L.H. and Kier, L.B., "The Molecular Connectivity Chi Indexes and Kappa Shape Indexes in Structure-Property Modeling," *Reviews in Computational Chemistry: Advances*, VCH Publishers, Inc., 1991, pp. 367-422.
	AP	5	Hecht-Nielsen, R., "Replicator Neural Networks for Universal Optimal Source Coding," *Science*, American Association for the Advancement of Science, Vol. 269, September 29, 1995, pp. 1860-1863.
	AQ	5	Hotelling, H., "Analysis of a Complex of Statistical Variables into Principal Components," *The Journal of Educational Psychology*, Warwick and York, Inc., Vol. XXIV, No. 6, September 1933, pp. 417-441.
	AR	5	Hotelling, H., "Analysis of a Complex of Statistical Variables into Principal Components," *The Journal of Educational Psychology*, Warwick and York, Inc., Vol. XXIV, No. 7, October 1933, pp. 498-520.

EXAMINER [signature] DATE CONSIDERED 24JAN04

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	AA6						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ6						No
	AK6						Yes No
	AL6						Yes No
	AM6						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	6	Lee, R.C.T. *et al.*, "A Triangulation Method for the Sequential Mapping of Points from *N*-Space to Two-Space," *IEEE Transactions on Computers*, The Institute of Electrical and Electronics Engineers, March 1977, pp. 288-292.
	AO	6	Lipinski, C.A. *et al.*, "Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings," *Advanced Drug Delivery Reviews*, Elsevier Science B.V., Vol. 23, 1997, pp. 3-25.
	AP	6	Lobanov, V.S. and Agrafiotis, D.K., "Intelligent Database Mining Techniques," *Abstracts of Papers Part 1: 215th ACS National Meeting*, March 29-April 2, 1998, p. 19-COMP.
	AQ	6	Lobanov, V.S. *et al.*, "Rational Selections from Virtual Libraries," *Abstracts of Papers Part 1: 217th ACS National Meeting*, March 21-25, 1999, p. 181-COMP.
	AR	6	Mao, J. and Jain, A.K., "Artificial Neural Networks for Feature Extraction and Multivariate Data Projection," *IEEE transactions on Neural Networks*, IEEE Neural Networks Council, Vol. 6, No. 2, March 1995, pp. 296-317.

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ7						Yes No
	AK7						No
	AL7						Yes No
	AM7						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	7	Oja, E., "Principal Components, Minor Components, and Linear Neural Networks," *Neural Networks*, Pergamon Press Ltd., Vol. 5, 1992, pp. 927-935.
	AO	7	Patterson, D.E. *et al.*, "Neighborhood Behavior: A Useful Concept for Validation of 'Molecular Diversity' Descriptors," *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 39, No. 16, 1996, pp. 3049-3059.
	AP	7	Pykett, C.E., "Improving the Efficiency of Sammon's Nonlinear Mapping by Using Clustering Archetypes," *Electronics Letters*, The Institution of Electrical Engineers, Vol. 14, No. 25, December 7, 1978, pp. 799-800.
	AQ	7	Rubner, J. and Tavan, P., "A Self-Organizing Network for Principal-Component Analysis," *Europhysics Letters*, European Physical Society, Vol. 10, No. 7, December 1, 1989, pp. 693-698.
	AR	7	Sadowski, J. *et al.*, "Assessing Similarity and Diversity of Combinatorial Libraries by Spatial Autocorrelation Functions and Neural Networks," *Angewandte Chemie*, VCH, Vol. 34, No. 23/24, January 5, 1996, pp. 2674-2677.

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	AA8						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ8						No
	AK8						No
	AL8						No
	AM8						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	8	Thompson, L.A. and Ellman, J.A., "Synthesis and Applications of Small Molecule Libraries," *Chemical Reviews*, American Chemical Society, Vol. 96, No. 1, January/February 1996, pp. 555-585, 588-600.
	AO	8	Barnard, John M. and Downs, Geoff M., "Computer representation and manipulation of combinatorial libraries," *Perspectives in Drug Discovery and Design*, Kluwer Academic Publishers, 1997, pp. 13-30.
	AP	8	Brint, Andrew T. and Willett, Peter, "Upperbound procedures for the identification of similar three-dimensional chemical structures," *Journal of Computer-Aided Molecular Design*, ESCOM Science Publishers B.V., Vol. 2, No. 4, January 1989, pp. 311-320.
	AQ	8	Brown, Robert D. and Martin, Yvonne C., "Designing Combinatorial Library Mixtures Using a Genetic Algorithm," *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 40, No. 15, 1997, pp. 2304-2313.
	AR	8	Gillet, Valerie J. *et al.*, "The Effectiveness of Reactant Pools for Generating Structurally-Diverse Combinatorial Libraries," *Journal of Chemical and Information Computer Sciences*, American Chemical Society, Vol. 37, No. 4, 1997, pp. 731-740.

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	AA9						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ9						Yes No
	AK9						Yes No
	AL9						Yes No
	AM9						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	9	Gillet, Valerie J. *et al.*, "Selecting Combinatorial Libraries to Optimize Diversity and Physical Properties," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 39, No. 1, December 17, 1998 (Published on Web), pp. 169-177.
	AO	9	Kearsley, Simon K. *et al.*, "Chemical Similarity Using Physiochemical Property Descriptors," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 36, No. 1, 1996, pp. 118-127.
	AP	9	Leland, Burton A. *et al.*, "Managing the Combinatorial Explosion," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 37, No. 1, 1997, pp. 62-70.
	AQ	9	Lewis, Richard A. *et al.*, "Similarity Measures for Rational Set Selection and Analysis of Combinatorial Libraries: The Diverse Property-Derived (DPD) Approach," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 37, No. 3, 1997, pp. 599-614.
	AR	9	Martin, Eric J. and Critchlow, Roger E., "Beyond Mere Diversity: Tailoring Combinatorial Libraries for Drug Discovery," *Journal of Combinatorial Chemistry*, American Chemical Society, Vol. 1, No. 1, December 18, 1998 (Published on Web), pp. 32-45.

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA10						
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ10						Yes No
	AK10						Yes No
	AL10						Yes No
	AM10						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	10	Sheridan, Robert P. *et al.*, "Chemical Similarity Using Geometric Atom Pair Descriptors," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 36, No. 1, 1996, pp. 128-136.
	AO	10	Willett, Peter *et al.*, "Chemical Similarity Searching," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 38, No. 6, July 21, 1998 (Published on Web), pp. 983-996.
	AP	10	Agrafiotis, Dimitris K. and Lobanov, Victor S., "Ultrafast Algorithm for Designing Focused Combinational Arrays," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, 2000, Vol. 40, No. 4, pp. 1030-1038.
	AQ	10	Ajay *et al.*, "Can We Learn To Distinguish between 'Drug-Like' and 'Nondrug-like' Molecules?" *Journal of Medicinal Chemistry*, July 23, 1998 (Published on Web), American Chemical Society, Vol. 41, No. 18, pp. 3314-3324.
	AR	10	English-language Abstract of European Patent No. 0 355 628, printed from Dialog File No. 351(February, 1990 - Date of publication of application), 2 pages.

EXAMINER	DATE CONSIDERED 24JAN04

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FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0930001	APPLICATION NO. 09/823,977
	APPLICANT Agrafiotis *et al.*	
	FILING DATE April 3, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ11						Yes No
	AK11						Yes No
	AL11						Yes No
	AM11						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	11	Brown, Robert D. and Martin, Yvonne C., "The Information Content of 2D and 3D Structural Descriptors Relevant to Ligand-Receptor Binding," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, 1997, Vol. 37, No. 1, pp. 1-9.
	AO	11	Brown, Robert D. and Martin, Yvonne C., "Use of Structure-Activity Data To Compare Structure-Based Clustering Methods and Descriptors for Use in Compound Selection," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, 1996, Vol. 36, No. 3, pp. 572-584.
	AP	11	Cummins, David J. *et al.*, "Molecular Diversity in Chemical Databases: Comparison of Medicinal Chemistry Knowledge Bases and Databases of Commercially Available Compounds," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, 1996, Vol. 36, No. 4, pp. 750-763.
	AQ	11	Domine, D. *et al.*, "Non-Linear Mapping for Structure-Activity and Structure-Property Modelling," *Journal of Chemometrics*, John Wiley & Sons, Ltd., Vol. 7, No. 4, July-August 1993, pp. 227-242.
	AR	11	Rotstein, S.H. and Murcko, M., "GroupBuild: A Fragment-Based Method for *De Novo* Drug Design," *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 36, No. 12, 1993, pages 1700-1710.

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	AN	12	Downs, Geoff M. and Barnard, John M., "Techniques for Generating Descriptive Fingerprints in Combinatorial Libraries," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, 1997, Vol. 37, No. 1, pp. 59-61.
	AO	12	Gillet, Valerie J., "Background Theory of Molecular Diversity," *Molecular Diversity in Drug Design*, Kluwer Academic Publishers, 1999, pp. 43-65.
	AP	12	Good, Andrew C. and Lewis, Richard A., "New Methodology for Profiling Combinatorial Libraries and Screening Sets: Cleaning Up the Design Process with HARPick," *Journal of Medicinal Chemistry*, American Chemical Society, 1997, Vol. 40, No. 24, pp. 3926-3936.
	AQ	12	Pal, N.R. and Eluri, V.K., "Two Efficient Connectionist Schemes for Structure Preserving Dimensionality Reduction," *IEEE Transactions on Neural Networks*, IEEE, Vol 9, No. 6, November 1998, pp. 1142-1154.
	AR	12	Jamois, Eric A. *et al.*, "Evaluation of Reagent-Based and Product-Based Strategies in the Design of Combinatorial Library Subsets," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, December 9, 1999 (Published on Web), Vol. 40, No.1, pp. 63-70.

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	APPLICANT Agrafiotis *et al.*	
	FILING DATE April 3, 2001	GROUP 2122

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OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	13	Kim, H. *et al.*, "Self-Organized Distributed Networks for Learning Highly Nonlinear Mapping," *Intelligent Engineering Systems Through Artificial Neural Networks*, American Society of Mechanical Engineers, Vol. 4, 1994, pp. 109-114.
	AO	13	Leach, Andrew R. *et al.*, "Implementation of a System for Reagent Selection and Library Enumeration, Profiling, and Design," *Jounal of Chemical Information and Computer Sciences*, American Chemical Society, 1999, Vol. 39, No. 6, pp. 1161-1172.
	AP	13	Lobanov, Victor S. and Agrafiotis, Dimitris K., "Stochastic Similarity Selections from Large Combinatorial Libraries," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, January 21, 2000 (Published on Web), Vol. 40, No. 2, pp. 460-470.
	AQ	13	Matter, Hans and Pötter, Thorsten, "Comparing 3D Pharmacophore Triplets and 2D Fingerprints for Selecting Diverse Compound Subsets," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, October 29, 1999 (Published on Web), Vol. 39, No. 6, pp. 1211-1225.
	AR	13	Matter, Hans, "Selecting Optimally Diverse Compounds from Structure Databases: A Validation Study of Two-Dimensional and Three-Dimensional Molecular Descriptors," *Journal of Medicinal Chemistry*, American Chemical Society, 1997, Vol. 40, No. 8, pp. 1219-1229.

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	APPLICANT Agrafiotis *et al.*	
	FILING DATE April 3, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ14						No
	AK14						No
	AL14						No
	AM14						No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	14	Sadowski, Jens and Kubinyi, Hugo, "A Scoring Scheme for Discriminating between Drugs and Nondrugs," *Journal of Medicinal Chemistry*, American Chemical Society, August 1, 1998 (Published on Web), Vol. 41, No. 18, pp. 3325-3329.
	AO	14	Schnur, Dora, "Design and Diversity Analysis of Large Combinatorial Libraries Using Cell-Based Methods," *Journal of Chemical Information and Computer Science*, American Chemical Society, January 6, 1999 (Published on Web), Vol. 39, No. 1, pp. 36-45.
	AP	14	Schuffenhauer, Ansgar *et al.*, "Similarity Searching in Files of Three-Dimensional Chemical Structures: Analysis of the BIOSTER Database Using Two-Dimensional Fingerprints and Molecular Field Descriptors," *Journal of Chemical Information and Computer Science*, American Chemical Society, December 22, 1999 (Published on Web), Vol. 40, No. 2, pp. 295-307.
	AQ	14	Turner, David B. *et al.*, "Rapid Quantification of Molecular Diversity for Selective Database Acquisition," *Journal of Chemical Information and Computer Science*, American Chemical Society, 1997, Vol. 37, No. 1, pp. 18-22.
	AR	14	Wang, Jing and Ramnarayan, Kal, "Toward Designing Drug-Like Libraries: A Novel Computational Approach for Prediction of Drug Feasibility of Compounds," *Journal of Combinatorial Chemistry*, American Chemical Society, October 19, 1999 (Published on Web), Vol. 1, No. 6, pp. 524-533.

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	APPLICANT Agrafiotis *et al.*	
	FILING DATE April 3, 2001	GROUP 2122

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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ15						No
	AK15						No
	AL15						No
	AM15						No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	15	Gasteiger, J. *et al*, "Assessment of the Diversity of Combinatorial Libraries by an Encoding of Molecular Surface Properties," *Abstracts of Papers Part 1: 211th ACS National Meeting*, March 24-28, 1996, p. 70-CINF.
	AO	15	Hassan, Moises *et al.*, "Optimization and visualization of molecular diversity of combinatorial libraries," *Molecular Diversity*, ESCOM Science Publishers B.V., 1996, Vol. 2, No. 1/2, pp. 64-74.
	AP	15	Bellman, R.E., *Adaptive Control Processes: A Guided Tour*, Princeton Univ. Press, Princeton, NJ (1961), entire book submitted.
	AQ	15	Bezdek, J.C., *Pattern Recognition with Fuzzy Objective Function Algorithms*, Plenum Press, New York, NY (1981), entire book submitted.
	AR	15	Johnson, M.A., and Maggiora, G.M., *Concepts and Applications of Molecular Similarity*, John Wiley and Sons, New York, NY (1990), entire book submitted.

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U.S. PATENT DOCUMENTS

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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ16						No
	AK16						No
	AL16						No
	AM16						No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	16	Kohonen, T., *Self-Organizing Maps*, Springer-Verlag, Berlin, Germany (1995), entire book submitted.
	AO	16	Oja, E., *Subspace Methods of Pattern Recognition*, Research Studies Press Ltd., Letchworth, England (1983), entire book submitted.
	AP	16	Agrafiotis, D.K., "A New Method For Analyzing Protein Sequence Relationships Based On Sammon Maps," *Protein Science*, Cambridge University Press, Vol. 6, No. 2, February 1997, pp. 287-293.
	AQ	16	Copy of International Search Report issued October 18, 1999, for Appl. No. PCT/US99/09963, 7 pages.
	AR	16	Amzel, L.M., "Structure-based drug design," *Current Opinion in Biotechnology*, Vol. 9, No. 4, August 1998, pp. 366-369.

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ17						No
	AK17						No
	AL17						No
	AM17						No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	17	Blaney, J.M. and Martin, E.J., "Computational approaches for combinatorial library design and molecular diversity analysis," *Current Opinion in Chemical Biology*, Current Biology Ltd., Vol. 1, No. 1, June 1997, pp. 54-59.
	AO	17	Brown, R.D. and Clark, D.E., "Genetic diversity: applications of evolutionary algorithms to combinatorial library design," *Expert Opinion on Therapeutic Patents*, Vol. 8, No. 11, November 1998, pp. 1447-1459.
	AP	17	Caflisch, A. and Karplus, M., "Computational combinatorial chemistry for de novo ligand design: Review and assessment," *Perspectives in Drug Discovery and Design*, ESCOM Science Publishers B.V., Vol. 3, 1995, pp. 51-84.
	AQ	17	Danheiser, S.L., "Current Trends in Synthetic Peptide and Chemical Diversity Library Design," *Genetic Engineering News*, May 1, 1994, pp. 10 and 31.
	AR	17	Eichler, U. *et al.*, "Addressing the problem of molecular diversity," *Drugs of the Future*, Prous Science, Vol. 24, No. 2, 1999, pp. 177-190.

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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ18						Yes No
	AK18						Yes No
	AL18						Yes No
	AM18						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	18	Felder, E.R. and Poppinger, D., "Combinatorial Compound Libraries for Enhanced Drug Discovery Approaches," *Advances in Drug Research*, Academic Press, Vol. 30, 1997, pp. 112-199.
	AO	18	Geysen, H.M. and Mason, T.J., "Screening Chemically Synthesized Peptide Libraries for Biologically-Relevant Molecules," *Bioorganic & Medicinal Chemistry Letters*, Pergamon Press Ltd., Vol. 3, No. 3, 1993, pp. 397-404.
	AP	18	Gobbi, A. *et al.*, "New Leads By Selective Screening of Compounds From Large Databases," *Abstracts of Papers Part 1: 213th ACS National Meeting*, American Chemical Society, April 13-17, 1997, p. 67-CINF.
	AQ	18	Houghten, R.A. *et al.*, "The Use of Synthetic Peptide Combinatorial Libraries for the Identification of Bioactive Peptides," *Peptide Research*, Vol. 5, No. 6, 1992, pp. 351-358.
	AR	18	Klopman, G., "Artificial Intelligence Approach to Structure-Activity Studies. Computer Automated Structure Evaluation of Biological Activity of Organic Molecules," *Journal of the American Chemical Society*, American Chemical Society, Vol. 106, No. 24, 1984, pp. 7315-7321.

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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ19						Yes No
	AK19						Yes No
	AL19						Yes No
	AM19						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	19	Lajiness, M.S. *et al.*, "Implementing Drug Screening Programs Using Molecular Similarity Methods," *QSAR: Quantitative Structure-Activity Relationships in Drug Design*, Alan R. Liss, Inc., 1989, pp. 173-176.
	AO	19	Loew, G.H. *et al.*, "Strategies for Indirect Computer-Aided Drug Design," *Pharmaceutical Research*, Plenum Publishing Corporation, Vol. 10, No. 4, 1993, pp. 475-486.
	AP	19	Lynch, M.F. *et al.*, "Generic Structure Storage and Retrieval," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 25, No. 3, August 1985, pp. 264-270.
	AQ	19	Myers, P.L. *et al.*, "Rapid, Reliable Drug Discovery," *Today's Chemist At Work*, American Chemical Society, Vol. 6, No. 7, July/August 1997, pp. 46-48, 51 & 53.
	AR	19	Pabo, C.O. and Suchanek, E.G., "Computer-Aided Model-Building Strategies for Protein Design," *Biochemistry*, American Chemical Society, Vol. 25, No. 20, 1986, pp. 5987-5991.

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	AJ20						Yes No
	AK20						Yes No
	AL20						Yes No
	AM20						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	20	Saudek, V. *et al.*, "Solution Conformation of Endothelin-1 by H NMR, CD, and Molecular Modeling," *International Journal of Peptide Protein Research*, Munksgaard International Publishers Ltd., Vol. 37, No. 3, 1991, pp. 174-179.
	AO	20	Singh, J. *et al.*, "Application of Genetic Algorithms to Combinatorial Synthesis: A Computational Approach to Lead Identification and Lead Optimization," *J. Am. Chem. Soc.*, American Chemical Society, Vol. 118, No. 7, February 7, 1996, pp. 1669-1676.
	AP	20	Van Drie, J.H. and Lajiness, M.S., "Approaches to virtual library design," *Drug Discovery today*, Elsevier Science Ltd., Vol. 3, No. 6, June 1998, pp. 274-283.
	AQ	20	Walters, W.P. *et al.*, "Virtual screening - an overview," *Drug Discovery today*, Elsevier Science Ltd., Vol. 3, No. 4, April 1998, pp. 160-178.
	AR	20	Weber, L., "Evolutionary combinatorial chemistry: application of genetic algorithms," *Drug Discovery today*, Elsevier Science Ltd., Vol. 3, No. 8, August 1998, pp. 379-385.

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	AJ21						Yes No
	AK21						Yes No
	AL21						Yes No
	AM21						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	21	Weber, L. *et al.*, "Optimization of the Biological Activity of Combinatorial Compound Libraries by a Genetic Algorithm," *Angewandte Chemie International Edition in English*, VCH, Vol. 34, No. 20, November 3, 1995, pp. 2280-2282.
	AO	21	Graybill, T.L. *et al.*, "Enhancing the Drug Discovery Process by Integration of High-Throughput Chemistry and Structure-Based Drug Design," Molecular Diversity and Combinatorial Chemistry: Libraries and Drug Discovery, American Chemical Society, 1996, pp. 16-27.
	AP	21	Saund, E., "Dimensionality-Reduction Using Connectionist Networks," *IEEE Transactions on Pattern Analysis and Machine Intelligence*, IEEE, Vol. 11, No. 3, March 1989, pp. 304-314.
	AQ	21	"3DP gains drug research patent", *Chemistry in Britain*, The Royal Society of Chemistry, Vol. 32, No. 1, January 1996, p. 22.
	AR	21	"Accelerate the Discovery Cycle with Chem-X!", Source and date of publication unclear, 2 pages.

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	AJ22						Yes No
	AK22						Yes No
	AL22						Yes No
	AM22						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	22	Agrafiotis, D. K., "Stochastic Algorithms for Maximizing Molecular Diversity", *Journal of Chemical Information and Computer Sciences,* American Chemical Society, Vol. 37, No. 5, 1997, pp. 841-851.
	AO	22	Alsberg, B.K. *et al.*, "Classification of pyrolysis mass spectra by fuzzy multivariate rule induction-comparison with regression, *K*-nearest neighbour, neural and decision-tree methods", *Analytica Chimica Acta*, Elsevier Science B.V., Vol. 348, No. 1-3, August 20, 1997, pp. 389-407.
	AP	22	Andrea, T.A. and Kalayeh, H., "Applications of Neural Networks in Quantitative Structure-Activity Relationships of Dihydrofolate Reductase Inhibitors", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 34, No. 9, 1991, pp. 2824-2836.
	AQ	22	Aoyama, T. *et al.*, "Neural Networks Applied to Quantitative Structure-Activity Relationship", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 33, No. 3, 1990, pp. 905-908.
	AR	22	Aoyama, T. and Ichikawa, H., "Obtaining the Correlation Indices between Drug Activity and Structural Parameters Using a Neural Network", *Chemical & Pharmaceutical Bulletin*, Pharmaceutical Society of Japan, Vol. 39, No. 2, February 1991, pp. 372-378.

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FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0930001	APPLICATION NO. 09/823,977
	APPLICANT Agrafiotis *et al.*	
	FILING DATE April 3, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA23						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ23						Yes No
	AK23						Yes No
	AL23						Yes No
	AM23						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	23	"ArQule Inc", from *http://www.bioportfolio.com/arqule/products.htm*, 5 pages, (March 18, 1998).
	AO	23	Baum, R.M., "Combinatorial Approaches Provide Fresh Leads for Medicinal Chemistry", *Chemical & Engineering News*, American Chemical Society, February 7, 1994, pp. 20-26.
	AP	23	Bentley, J. L., "Multidimensional Binary Search Trees Used for Associative Searching", *Communications of the ACM*, Association for Computing Machinery, Inc., Vol. 18, No. 9, September 1975, pp. 509-517.
	AQ	23	Bottou, L. and Vapnik, V. "Local Learning Algorithms", *Neural Computation*, Massachusetts Institute of Technology, Vol. 4, No. 6, November 1992, pp. 888-900.
	AR	23	Boulu, L.G. and Crippen, G.M., "Voronoi Binding Site Models: Calculation of Binding Modes and Influence of Drug Binding Data Accuracy", *Journal of Computational Chemistry*, John Wiley & Sons, Inc., Vol. 10, No. 5, July/August 1989, pp. 673-682.

EXAMINER	DATE CONSIDERED 24 Jan 04

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	APPLICANT Agrafiotis *et al.*	
	FILING DATE April 3, 2001	GROUP 2122

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA24						
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ24						Yes No
	AK24						Yes No
	AL24						Yes No
	AM24						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	24	Boulu, L.G. *et al.*, "Voronoi Binding Site Model of a Polycyclic Aromatic Hydrocarbon Binding Protein", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 33, No. 2, 1990, pp. 771-775.
	AO	24	Cacoullos, T., "Estimation of a Multivariate Density", *Annals of The Institute of Statistical Mathematics*, The Institute of Statistical Mathematics, Vol. 18, No. 2, 1966, pp. 179-189.
	AP	24	Clark, R.D., "OptiSim: An Extended Dissimilarity Selection Method for Finding Diverse Representative Subsets", *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 37, No. 6, 1997, pp. 1181-1188.
	AQ	24	Clark, D. E., and Westhead, D.R., "Evolutionary algorithms in computer-aided molecular design", *Journal of Computer-Aided Molecular Design*, ESCOM Science Publishers B.V., Vol. 10, No. 4, August 1996, pp. 337-358.
	AR	24	Cramer, III, R. D. *et al.*, "Comparative Molecular Field Analysis (CoMFA). 1. Effect of Shape on Binding of Steroids to Carrier Proteins", *Journal of The American Chemical Society*, American Chemical Society, Vol. 110, No. 18, August 31, 1988, pp. 5959-5967.

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	APPLICANT Agrafiotis *et al.*	
	FILING DATE April 3, 2001	GROUP 2122

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	AJ25						Yes No
	AK25						Yes No
	AL25						Yes No
	AM25						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	25	Cramer, III, R. D. *et al.*, "Substructural Analysis. A Novel Approach to the Problem of Drug Design", *Journal of Medicinal Chemistry*, Vol. 17, No. 5, May 1974, pp. 533-535.
	AO	25	Crippen, G. M., "Voronoi Binding Site Models", *Journal of Computational Chemistry*, John Wiley & Sons, Inc., Vol. 8, No. 7, October/November 1987, pp. 943-955.
	AP	25	Friedman, J. H. *et al.*, "An Algorithm for Finding Best Matches in Logarithmic Expected Time", *ACM Transactions on Mathematical Software*, Association for Computing Machinery, Vol. 3, No. 3, September 1977, pp. 209-226.
	AQ	25	Friedman, J.H., "Fitting Functions To Noisy Data In High Dimensions", Department of Statistics- Stanford University Technical Report No. 101, (August, 1988), pages 1-36.
	AR	25	Gallop, M. A. *et al.*, "Applications of Combinatorial Technologies to Drug Discovery. 1. Background and Peptide Combinatorial Libraries", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 37, No. 9, April 29, 1994, pp. 1233-1251.

EXAMINER	DATE CONSIDERED 24JA-04

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

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	APPLICANT Agrafiotis *et al.*	
	FILING DATE April 3, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ26						Yes No
	AK26						Yes No
	AL26						Yes No
	AM26						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	26	Ghose, A. K. and Crippen, G.M., "Use of Physicochemical Parameters in Distance Geometry and Related Three-Dimensional Quantitative Structure-Activity Relationships: A Demonstration Using *Escherichia coli* Dihydrofolate Reductase Inhibitors", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 28, No. 3, 1985, pp. 333-346.
	AO	26	Good, A. C. *et al.*, "Structure-Activity Relationships from Molecular Similarity Matrices", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 36, No. 4, February 19, 1993, pp. 433-438.
	AP	26	Gordon, E. M. *et al.*, "Applications of Combinatorial Technologies to Drug Discovery. 2. Combinatorial Organic Synthesis, Library Screening Strategies, and Future Directions", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 37, No. 10, May 13, 1994, pp. 1385-1401.
	AQ	26	Hartigan, J. A., "Representation of Similarity Matrices By Trees", *Journal of the American Statistical Association*, Vol. 62, No. 320, December, 1967, pp. 1140-1158.
	AR	26	Hopfinger, A. J., "A QSAR Investigation of Dihydrofolate Reductase Inhibition by Baker Triazines Based upon Molecular Shape Analysis", *Journal of the American Chemical Society*, American Chemical Society, Vol. 102, No. 24, November 19, 1980, pp. 7196-7206.

EXAMINER	DATE CONSIDERED
Silvia T. Fleetwood, Jr.	24 JAN 04

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	APPLICANT Agrafiotis *et al.*	
	FILING DATE April 3, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ27						Yes No
	AK27						Yes No
	AL27						Yes No
	AM27						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	27	Jackson, R. C., "Update on computer-aided drug design", *Current Opinion in BIOTECHNOLOGY*, Current Biology Ltd., Vol. 6, No. 6, December 1995, pp. 646-651.
	AO	27	Kim, K. H., "Comparative molecular field analysis (CoMFA)", *Molecular Similarity in Drug Design*, ed. P. M. Dean, Blackie Academic & Professional, 1995, Ch. 12, pp. 291-331.
	AP	27	Kohonen, T., "Self-Organized Formation of Topologically Correct Feature Maps", *Biological Cybernetics*, Springer-Verlag, Vol. 43, No. 1, 1982, pp. 59-69.
	AQ	27	Koile, K. and Shapiro, R., "Building A Collaborative Drug Design System", *Proceedings of the 25h Hawaii International Conference on System Sciences*, IEEE, 1992, pp. 706-716.
	AR	27	Kowalski, B. R. and Bender, C. F., "Pattern Recognition. II. Linear and Nonlinear Methods for Displaying Chemical Data", *Journal of the American Chemical Society*, American Chemical Society, Vol. 95, No. 3, February 7, 1973, pp. 686-693.

EXAMINER [signature] DATE CONSIDERED 24 JAN 04

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	APPLICANT Agrafiotis *et al.*	
	FILING DATE April 3, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ28						Yes No
	AK28						Yes No
	AL28						Yes No
	AM28						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	28	Kruskal, J. B., "Nonmetric Multidimensional Scaling: A Numerical Method", *Psychometrika*, Vol. 29, No. 2, June, 1964, pp. 115-129.
	AO	28	Lengauer, T. and Rarey, M., "Computational methods for biomolecular docking", *Current Opinion in Structural Biology*, Current Biology Ltd, Vol. 6, No. 3, June, 1996, pp. 402-406.
	AP	28	Luke, B. T., "Evolutionary Programming Applied to the Development of Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships", *Journal of Chemical Information and Computer Sciences,* American Chemical Society, Vol. 34, No. 6, November/December 1994, pp. 1279-1287.
	AQ	28	Martin, E. J. *et al.*, "Does Combinatorial Chemistry Obviate Computer-Aided Drug Design?", *Reviews in Computational Chemistry*, VCH Publishers, Inc., Vol. 10, 1997, pp. 75-99.
	AR	28	Martin, E. J. *et al.*, "Measuring Diversity: Experimental Design of Combinatorial Libraries for Drug Discovery", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 38, No. 9, April 28, 1995, pp. 1431-1436.

EXAMINER [signature] DATE CONSIDERED 2/5/04

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	APPLICANT Agrafiotis *et al.*	
	FILING DATE April 3, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ29						Yes No
	AK29						Yes No
	AL29						Yes No
	AM29						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	29	McMartin, C. and Bohacek, R.S., "QXP: Powerful, rapid computer algorithms for structure-based drug design", *Journal of Computer-Aided Molecular Design*, Kluwer Academic Publishers, Vol. 11, No. 4, July 1997, pp. 333-344.
	AO	29	Mezey, P. G. and Walker, P.D., "Fuzzy molecular fragments in drug research", *Drug Discovery today*, Vol. 2, No. 4, April 1997, pp. 132-137.
	AP	29	Müller, K., "On the paradigm shift from rational to random design", *Journal of Molecular Structure (Theochem)*, Elsevier Science B.V., Vol. 398-399, Special Issue, 1997, pp. 467-471.
	AQ	29	Myers, P., "The Design Of A Universal, Informer™ Library", COMBICHEM, INC., 10 Pages, Date unknown.
	AR	29	Oinuma, H. *et al.*, "Neural Networks Applied to Structure-Activity Relationships", *Journal of Medicinal Chemistry*, Vol. 33, No. 3, pp. 905-908, (1990).

EXAMINER	DATE CONSIDERED
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ30						Yes No
	AK30						Yes No
	AL30						Yes No
	AM30						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

WLG	AN	30	Omohundro, S. M., "Bumptrees for Efficient Function, Constraint, and Classification Learning", *Advances in Neural Information Processing Systems 3*, Morgan Kaufmann, 1991, 7 pages, unknown.
	AO	30	Parrill, A. L., "Evolutionary and genetic methods in drug design", *Drug Discovery today*, Elsevier Science Ltd., Vol. 1, No. 12, December 1996, pp. 514-521.
	AP	30	Polanski, J., "A neural network for the simulation of biological systems", *Journal of Molecular Structure (Theochem)*, Elsevier Science Ltd., Vol. 398-399, Special Issue, 1997, pp. 565-571.
	AQ	30	Ramos-Nino, M. E. *et al.*, "A comparison of quantitative structure-activity relationships for the effect of benzoic and cinnamic acids on *Listeria monocytogenes* using multiple linear regression, artificial neural network and fuzzy systems", *Journal of Applied Microbiology*, Society for Applied Bacteriology, Vol. 82, No. 2, February 1997, pp. 168-176.
	AR	30	Rogers, D. and Hopfinger, A. J., "Application of Genetic Function Approximation to Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships", *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 34, No. 4, July/August 1994, pp. 854-866.

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U.S. PATENT DOCUMENTS

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	AJ31						Yes No
	AK31						Yes No
	AL31						Yes No
	AM31						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	31	Sammon, Jr., J. W., "A Nonlinear Mapping for Data Structure Analysis", *IEEE Transactions on Computers*, IEEE, Vol. C-18, No. 5, May 1969, pp. 401-409.
	AO	31	Simon, Z. *et al.*, "Mapping of Dihydrofolate-reductase Receptor Site by Correlation with Minimal Topological (Steric) Differences", *Journal of Theoretical Biology*, Academic Press, Inc., Vol. 66, No. 3, June 7, 1997, pp. 485-495.
	AP	31	Smellie, A. S. *et al.*, "Fast Drug-Receptor Mapping by Site-Directed Distances: A Novel Method of Predicting New Pharmacological Leads", *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 31, No.3, August 1991, pp. 386-392.
	AQ	31	Specht, D. F., "A General Regression Neural Network", *IEEE Transactions on Neural Networks*, IEEE, Vol. 2, No. 6, November 1991, pp. 568-576.
	AR	31	Svozil, D. *et al.*, "Neural Network Prediction of the Solvatochromic Polarity/Polarizability Parameter π^H_2", *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 37, No. 2, 1997, pp. 338-342.

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FOREIGN PATENT DOCUMENTS

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	AJ32						Yes No
	AK32						Yes No
	AL32						Yes No
	AM32						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	32	Todorov, N. P. and Dean, P. M., "Evaluation of a method for controlling molecular scaffold diversity in de novo ligand design", *Journal of Computer-Aided Molecular Design*, ESCOM Science Publishers B.V., Vol. 11, 1997, pp. 175-192.
	AO	32	Torgerson, W. S., "Multidimensional Scaling: I. Theory and Method", *Psychometrika*, The Psychometric Society, Vol. 17, No. 4, December 1952, pp. 401-419.
	AP	32	Vapnik, V., "Principles of Risk Minimization for Learning Theory", *Advances in Neural Information Processing Systems 4*, Morgan Kaufmann Publishers, Inc., 1992, pp. 831-838.
	AQ	32	Vapnik, V. and Bottou, L., "Local Algorithms for Pattern Recognition and Dependencies Estimation", *Neural Computation*, Massachusetts Institute of Technology, Vol. 5, No. 6, November 1993, pp. 893-909.
	AR	32	Viswanadhan, V. N. *et al.*, "Mapping the binding site of the nucleoside transporter protein: a 3D-QSAR study", *Biochimica et Biophysica Acta*, Elsevier Science Publishers B.V., Vol. 1039, No. 3, 1990, pp. 356-366.

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	AJ33						Yes No
	AK33						Yes No
	AL33						Yes No
	AM33						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	33	Warr, W. A., "Exploiting Molecular Diversity: Small Molecule Libraries for Drug Discovery", Report of Conference held in La Jolla, California, Jan. 23-25, 1995.
	AO	33	Westhead, D. R. *et al.*, "A comparison of heuristic search algorithms for molecular docking", *Journal of Computer-Aided Molecular Design*, Kluwer Academic Publishers, Vol. 11, 1997, pp. 209-228.
	AP	33	Willett, P., "Genetic algorithms in molecular recognition and design", *Trends in Biotechnology*, Elsevier Science Publishers B.V., Vol, 13, No. 12, December 1995, pp. 516-521.
	AQ	33	Willett, P. and Winterman, V., "A Comparison of Some Measures for the Determination of Inter-Molecular Structural Similarity Measures of Inter-Molecular Structural Similarity", *Quantitative Structure-Activity Relationships*, VCH, Vol. 5, No. 1, March 1986, pp. 18-25.
	AR	33	Zadeh, L. A., "Communication Fuzzy Algorithms", *Information and Control*, Academic Press Inc., Vol. 12, No. 2, February 1968, pp. 94-102.

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U.S. PATENT DOCUMENTS

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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ34						Yes No
	AK34						Yes No
	AL34						Yes No
	AM34						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	34	Zadeh, L. A., "Fuzzy Sets", *Information and Control*, Academic Press Inc., Vol. 8, No. 3, June 1965, pp. 338-353.
	AO	34	Copy of International Search Report issued April 21, 1998 for Appl. No. PCT/US97/20919, 6 pages.
	AP	34	Copy of International Search Report issued May 13, 1998 for Appl. No. PCT/US97/20918, 7 pages.
	AQ	34	Aoyama, T. *et al.*, "Neural Networks Applied to Structure-Activity Relationships," *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 33., No. 3, 1990, pp. 2583-2590.
	AR	34	Gasteiger, J. *et al.*, "Analysis of the Reactivity of Single Bonds in Aliphatic Molecules by Statistical and Pattern Recognition Methods," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 33, No. 3, 1993, pp. 385-394.

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	FILING DATE April 3, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

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	AJ35						Yes No
	AK35						Yes No
	AL35						Yes No
	AM35						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	35	Guez, A. and Nevo, I., "Neural networks and fuzzy logic in clinical laboratory computing with application to integrated monitoring," *Clinica Chimica Acta*, Elsevier Science Publishers B.V., Vol. 248, 1996, pp. 73-90.
	AO	35	Rouvray, D.H., "Similarity in Chemistry: Past, Present and Future," *Topics in Chemistry*, Springer-Verlag, Vol. 173, 1995, pp. 1-30.
	AP	35	de Ridder, D. and Duin, R.P.W., "Sammon's mapping using neural networks: A comparison," *Pattern Recognition Letters*, Elsevier Science Publishers B.V., Vol. 18, No. 11-13, 1997, pp. 1307-1316.
	AQ	35	Copy of International Search Report issued September 24, 2001 for Appln. No. PCT/US01/06217, 3 pages.
	AR	35	Chang, G. et al., "An Internal Coordinate Monte Carlo Method for Searching Conformational Space, *Journal of the American Chemical Society*, American Chemical Society, Vol. III, June 1989, No. 12, pages 4379-4386.

EXAMINER	DATE CONSIDERED 24 JAN 04

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FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0930001	APPLICATION NO. 09/823,977
	APPLICANT Agrafiotis *et al.*	
	FILING DATE April 3, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA36						
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ36						Yes No
	AK36						Yes No
	AL36						Yes No
	AM36						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	36	Crippen, G.M. and Havel, T.F., *Distance Geometry and Molecular Conformation*, Research Studies Press Ltd., 1988, entire book submitted.
	AO	36	Feuston, B. *et al.*, "Comparison of Knowledge-Based and Distance Geometry Approaches for Generation of Molecular Conformations," *Journal of Information and Computer Sciences*, American Chemical Society, Vol. 41, No. 3, April 12, 2001 (Published on Web), pages 754-763.
	AP	36	Ferguson, D. and Raber, D., "A New Approach to Probing Conformational Space with Molecular Mechanics: Random Incremental Pulse Search," *Journal of the American Chemical Society*, American Chemical Society, Vol. 111, No. 12, 1989, pages 4371-4378.
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	AJ37						Yes No
	AK37						Yes No
	AL37						Yes No
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OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	37	Huang, E. *et al.*, "Distance geometry generates native-like folds for small helical proteins using the consensus distances of predicted protein structures," *Protein Science*, The Protein Society, Vol. 7, No. 9, September 1998, pages 1998-2003.
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	AR	37	Jain, A. and Mao, J., "Artificial Neural Networks: A Tutorial," IEEE, March 1996, pages 31-44.

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	AA38						
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	AJ38						Yes No
	AK38						Yes No
	AL38						Yes No
	AM38						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

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	AR	38	Mumenthaler, Ch. And Braun, W., "Automated Assignment of Simulated and Experimental NOESY Spectra of Proteins by Feedback Filtering and Self-correcting Distance Geometry," *Journal of Molecular Biology*, Academic Press Limited, Vol. 254, No. 3, December 1, 1995, pages 465-480.

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	AJ39						Yes No
	AK39						Yes No
	AL39						Yes No
	AM39						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	39	Porto, V.W. *et al.*, "Alternative Neural Network Training Methods," *IEEE Expert*, IEEE, Vol. 10, No. 4, June 1995, pages 16-22.
	AO	39	Saunders, M. , "Stochastic Exploration of Molecular Mechanics Energy Surfaces. Hunting for the Global Minimum," *Journal of the American Chemical Society*, American Chemical Society, Vol. 109, May 13, 1987, pages 3150-3152.
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	AA40						
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	AJ40						Yes No
	AK40						Yes No
	AL40						Yes No
	AM40						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AN	40	Cohen, N.C. *et al.*, "Molecular Modeling Software and Methods for Medicinal Chemistry," *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 33, No. 3, March 1990, pages 883-894.
	AO	40	Linusson, A. *et al.*, "Statistical Molecular Design of Building Blocks for Combinatorial Chemistry," *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 43, No. 7, March 8, 2000 (Published on Web), pages 1320-1328.
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